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Published in:
Journal of Applied Physics

DOI:
[10.1063/1.1522490](https://doi.org/10.1063/1.1522490)

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2003

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Citation for published version (APA):

Palasantzas, G., & De Hosson, J. T. M. (2003). Effect of roughness on the conductivity of semiconducting thin films/quantum wells with double rough boundaries. *Journal of Applied Physics*, 93(1), 320-324. <https://doi.org/10.1063/1.1522490>

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Effect of roughness on the conductivity of semiconducting thin films/quantum wells with double rough boundaries

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(Received 20 September 2002; accepted 27 September 2002)

We have investigated the influence of surface/interface roughness on the electrical conductivity in semiconducting thin films/quantum wells with double self-affine rough interface boundaries. The self-affine boundary roughness is characterized by the roughness exponent H , the in-plane correlation length ξ , and the rms amplitude Δ . In addition, nonzero cross correlation between the interfaces are taken into account during the conductivity calculations. The latter is shown to affect strongly the electrical conductivity. Nevertheless, the exact effect depends strongly on the values of the interface correlation lengths and roughness exponents. Finally, the ratio between conductivities slightly below and above the critical thickness for which the second miniband is occupied is shown to be strongly sensitive on the form of the correlation function (or the interface roughness exponents), and the presence of cross correlations. © 2003 American Institute of Physics.
[DOI: 10.1063/1.1522490]

I. INTRODUCTION

The electrical conductivity of thin semiconducting films limited by electron surface/interface scattering is a topic of broad interest over the last 15 years because of fundamental and technological importance in microelectronics devices.^{1–10} In silicon-metal-oxide semiconductor inversion layers (MOS) with high electron density ($>10^{-2} \text{ nm}^{-2}$), the low temperature mobility and conductivity of a two-dimensional electron gas are dominated by interfacial scattering.⁶ On the other hand, for single heterojunction systems (e.g., AlGaAs/GaAs) it has been predicted that the interface roughness scattering has only a minor influence on the carrier conductivity due to loose electron confinement,⁷ while the situation is different in thin quantum wells where small interface roughness could lead to strong electron scattering. In fact, in a AlGaAs/GaAs/AlGaAs quantum well the roughness scattering becomes important for GaAs well thickness less than 10 nm.^{8,9} Similar influence of interface roughness on electronic transport was also found in other systems, e.g., in HgTe–CdTe superlattices.¹⁰

Furthermore, the electrical conductivity σ of thin semiconducting films and quantum wells, whenever is limited by electron roughness scattering, has been shown to follow the power law $\sigma \propto d^6$ with d the film/well thickness.^{1–3} This result holds not only in the limit $k_F \xi \ll 1$, with k_F the Fermi wave vector and ξ the roughness in-plane correlation length, but also for $k_F \xi \gg 1$ (where the form of the interface roughness correlation function plays a significant role¹) if we properly consider dynamic roughness evolution effects on the electrical conduction.³ In addition, surface/interface roughness fractality effects (which are described by the roughness exponent H) were shown to have a significant influence on

the conductivity for both metallic and semiconducting films.^{4,5}

Within a similar framework, Fishman and Calecki¹ have shown that the form of the roughness correlation function has a significant influence on the ratio of electron conductivities for the Fermi level E_F , respectively, slightly below and above the second miniband edge. Indeed, in the limit $k_F \xi \ll 1$, the conductivity ratio acquires a constant value, while for $k_F \xi > 1$ it becomes highly sensitive to form of the roughness correlation. In these studies the conductivity (or mobility) ratio for the Gaussian correlation function $C(r) \sim \exp(-r^2/\xi^2)$ was found to be significantly different from the mobility ratio for simple exponential correlations $C(r) \sim \exp(-r/\xi)$; being typically larger in the former case for moderate correlation lengths ξ (smaller than half of the critical width above which the Fermi level crosses the second miniband).^{1,5} The previous correlation forms can be considered as special cases of surfaces/interfaces with fractality exponents $H=1$ and 0.5 if they are considered in terms of the stretched exponential correlation function $C(r) \sim e^{-(r/\xi)^{2H}}$ which has been used to model random thin film surface/interface roughness.¹¹ Surface/interface fractality exponents $H \geq 0$ were also shown to have significant impact on such conductivity ratio.⁵

Moreover, thin films can be bounded by interfaces that are both rough with a nonzero cross correlation between them. The latter effect has already been considered implicitly in conduction studies,¹² and studied explicitly for the case of thin metallic films.^{13,14} However, for semiconducting films/quantum wells, the influence of nonzero roughness cross correlation still remains unexplored. Therefore, in this work we shall address the influence of cross correlations for the case of semiconducting thin films/quantum wells bounded by correlated self-affine rough interfaces, which is the more general case of surface/interface roughness observed in thin films grown under nonequilibrium conditions.¹⁵

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II. CONDUCTIVITY THEORY

The bottom and top boundaries of the semiconducting film/quantum well are defined by the equations $z = -d/2 + h_1(r)$, and $z = d/2 + h_2(r)$, respectively. The roughness fluctuations $h_{1,2}(\mathbf{r})$ are assumed to be single-valued random functions of the in-plane position vector $\mathbf{r} = (x, y)$. Moreover, the roughness is assumed to be isotropic such that the height-height correlation functions depend only on the relative distance $r = |\mathbf{r}|$. During the conductivity calculations we assumed that the charge carrier motion is quantized along the z direction perpendicular to the film plane, while it remains free along the in-plane x and y directions.

Under the assumption that only surface/interface morphology contributes to the electron scattering (ignoring any volume impurities), the electrical conductivity σ is given in the Born approximation by the expression (see Appendix):^{3,13}

$$\sigma = \frac{e^2 \hbar^3}{m^2 d} \sum_{\nu=1}^N \sum_{\nu'=1}^N k_{\nu}^2 k_{\nu'}^2 \{ [C^{-1}(E_F)]_{\nu\nu'}^{\text{INC}} + [C^{-1}(E_F)]_{\nu\nu'}^{\text{COR}} \}, \quad (1)$$

$$C(E_F)_{\nu\nu'}^{\text{INC}} = \sum_{b=1}^2 \int_0^{2\pi} \left\{ \delta_{\nu\nu'} k_{\nu}^2 \left(\sum_{m=1}^N \tilde{A}_{\nu m}^b \langle |h_b(k_{m\nu})|^2 \rangle \right) - \tilde{A}_{\nu\nu'}^b k_{\nu} k_{\nu'} \langle |h_b(k_{m\nu})|^2 \rangle \cos \theta \right\} d\theta, \quad (2)$$

$$C(E_F)_{\nu\nu'}^{\text{COR}} = -2 \int_0^{2\pi} \left\{ \delta_{\nu\nu'} k_{\nu}^2 \left(\sum_{m=1}^N \tilde{B}_{\nu m} \langle |h_{12}(k_{m\nu})|^2 \rangle \right) - \tilde{B}_{\nu\nu'} k_{\nu} k_{\nu'} \langle |h_{12}(k_{m\nu})|^2 \rangle \cos \theta \right\} d\theta, \quad (3)$$

where $C(E_F)_{\nu\nu'}^{\text{INC}}$ is the incoherent component due to independent scattering from both interfaces, and $C(E_F)_{\nu\nu'}^{\text{COR}}$ the coherent component due to cross correlations among roughness fluctuations between consecutive interfaces. If the electrons are localized (for simplicity) by an infinite confining potential well we have $E_{\nu} = (\hbar^2/2m)(\nu\pi/d)^2$, $A_{\nu}^b = \hbar^2 \pi^2 \nu^2 / m d^3$, $B_{\nu} = (-1)^{1+\nu} \hbar^2 \pi^2 \nu^2 / m d^3$, $\tilde{A}_{\nu m}^b = A_{\nu}^b A_m^b$, and $\tilde{B}_{\nu m} = B_{\nu} B_m$. $\langle |h_b(k)|^2 \rangle$ is the Fourier transform of the height-height correlation function $C_b(r) = \langle h_b(\mathbf{r}) h_b(\mathbf{0}) \rangle$ ($b = 1, 2$), and $\langle |h_{12}(k)|^2 \rangle$ is the Fourier transform of the cross-correlation function $C_{12}(r) = \langle h_1(\mathbf{r}) h_2(\mathbf{0}) \rangle$ between interfaces indexed as 1 and 2. Finally, N is the number of occupied minibands, and $k_{\nu} = [(2m/\hbar^2)(E_F - E_{\nu})]^{1/2}$ with E_F and E_{ν} being, respectively, the Fermi energy and the energy minimum of the ν miniband (miniband edge) and $k_{\nu\nu'} = (k_{\nu}^2 + k_{\nu'}^2 - 2k_{\nu} k_{\nu'} \cos \theta)^{1/2}$. For a film of given thickness d and carrier density n , E_F , and N are determined by the condition $nd = (m/\pi \hbar^2)(NE_F - \sum_{\nu=1, N} E_{\nu}) \times (E_N \leq E_F)$.³⁻⁵

III. INTERFACE ROUGHNESS MODEL

In the following both rough interfaces will be modeled as self-affine rough interfaces that are widely observed to

occur for thin film surfaces/interfaces grown under nonequilibrium conditions.^{15,16} For self-affine roughness, the roughness-spectrum $\langle |h(k)|^2 \rangle$ scales as (Ref. 15) $\langle |h(k)|^2 \rangle \propto k^{-2-2H}$ if $k\xi \gg 1$ and $\langle |h(k)|^2 \rangle \propto \text{const}$ if $k\xi \ll 1$. The roughness exponent H is a measure of the degree of interface irregularity^{15,16} such that small values ($H \sim 0$) characterize jagged or irregular surfaces at small length scales ($< \xi$), while large values ($H \sim 1$) to smoother surfaces at $r < \xi$. The self-affine asymptotic limits of $\langle |h(k)|^2 \rangle$ are satisfied by the simple Lorentzian model:¹⁶

$$\langle |h(k)|^2 \rangle = (2\pi) \frac{w^2 \xi^2}{(1 + ak^2 \xi^2)^{1+H}}, \quad (4)$$

with $a = (1/2H)[1 - (1 + aQ_c^2 \xi^2)^{-H}]$ if $0 < H < 1$, and $a = (1/2)\ln(1 + aQ_c^2 \xi^2)$ if $H = 0$ (logarithmic roughness).¹⁶ $Q_c = \pi/a_o$ with a_o (≈ 0.3 nm) to the order of the atomic spacing. Furthermore, the cross-correlation term $\langle |h_{12}(k)|^2 \rangle$ will be considered in the form

$$\langle |h_{12}(k)|^2 \rangle = [\langle |h_1(k)|^2 \rangle \langle |h_2(k)|^2 \rangle]^{1/2} e^{-d/\tau}, \quad (5)$$

with τ a vertical cross-correlation length. Indeed, the form of Eq. (5) in Fourier space is inspired by the corresponding form of the real space cross-correlation function $C_{12}(r) = [C_1(r)C_2(r)]^{1/2} \exp(-d/\tau)$ that is widely used in the analysis of multilayer interface roughness in terms of x-ray scattering reflectivity measurements.¹⁷

IV. RESULTS FOR SEMICONDUCTING FILMS/QUANTUM WELLS

For semiconducting films/quantum wells the areal electron density $n_s (=nd)$ can be rather low so that the number of occupied minibands is also small ($N \leq 2$). Our calculations were performed for constant electron areal density $n_s = 4.8 \times 10^{-2} \text{ nm}^{-2}$, and constant rms roughness amplitudes for both rough interfaces $\Delta_{1,2} = 0.5$ nm such that $\Delta_{1,2} \ll d$ in order that the Born approximation for the conductivity to be valid.² Note that for the chosen value of n_s the critical thickness d_c above which the Fermi level E_F crosses the bottom of the second miniband ($N=2$) has the value $d_c = 10$ nm.

A. One miniband occupied ($N=1$)

For moderate thickness $d < d_c$ only one lateral miniband is occupied ($N=1$) which will be the case in the following if not stated otherwise. For $N=1$ the conductivity is given by

$$\sigma(d) = G_o \frac{4n_s d^5}{\pi^2} \left[\int_0^{2\pi} (\langle |h_1(q)|^2 \rangle + \langle |h_2(q)|^2 \rangle - 2\langle |h_{12}(q)|^2 \rangle (1 - \cos \theta) d\theta) \right]^{-1}, \quad (6)$$

with $G_o = e^2/2\pi \hbar$ and $q = [4\pi n_s(1 - \cos \theta)]^{1/2}$. Equation (6) shows that the spatial frequency regime of the interface morphology with wave vectors $0 < k < q_c = (8\pi n_s)^{1/2}$ will contribute to the film conductivity. This is due to the fact that forward scattering which contributes less to the conductivity occurs for $\theta = 0$ or 2π yielding $k_{11} = 0$, while backward scattering which has the largest contribution to the conductivity occurs for $\theta = \pi$ yielding $k_{11} = q_c = (8\pi n_s)^{1/2}$.

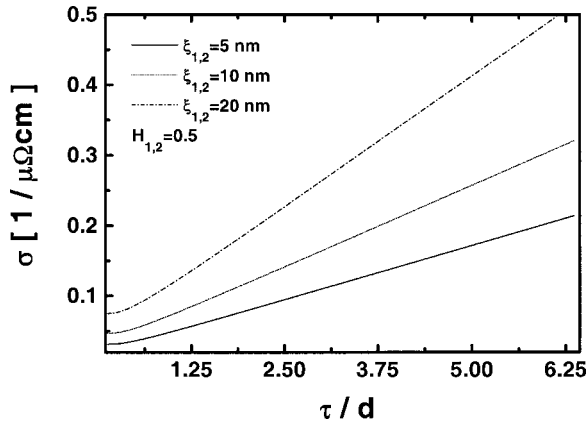


FIG. 1. Conductivity σ vs cross-correlation length τ for various interface correlation lengths $\xi_{1,2}$, $d=8$ nm, and interface exponents $H_{1,2}=0.5$.

Equation (6) clearly indicates that the presence of cross correlations will increase the film/well conductivity. This is clearly evident in Fig. 1 which shows the conductivity dependence on the cross-correlation length τ (rescaled with respect to film/well thickness d), where with increasing τ the effect of the cross correlation increases leading to conductivity enhancement. As the correlation lengths $\xi_{1,2}$ increase resulting in interface smoothening at long roughness wavelengths (since $\Delta_{1,2}/\xi_{1,2}$ decreases), electron scattering decreases leading thus to a higher conductivity and more significant cross-correlation effects. Similar is the behavior of the conductivity as the interface roughness exponents $H_{1,2}$ increase (Fig. 2) since the latter leads to interface smoothening at short roughness wavelengths ($r < \xi_{1,2}$) and thus to higher conductivity.

As a function of variable interface correlation length ξ_2 the conductivity σ has a minimum at $\xi_2 \approx \lambda_F/4$ ($\lambda_F \approx d$). This is displayed in Fig. 3. σ increases with increasing ξ_2 as was also observed in former studies.¹⁻⁴ The extreme behavior (minimum at $\xi_2 \approx \lambda_F/4$) is a result of the fact that interface roughness scatters effectively over finite length scales ($< \xi_{1,2}$). This is reflected by the fact that for small $\xi_{1,2}$ (and fixed wave vector q) we have $\langle |h_{1,2}(q)|^2 \rangle \propto \xi_{1,2}^2$ and there-

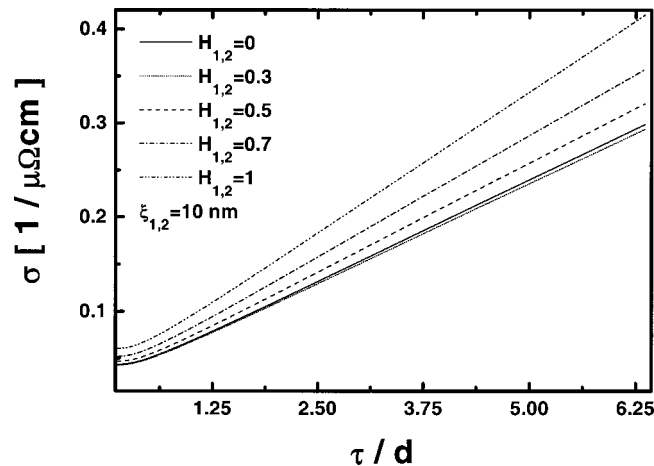


FIG. 2. Conductivity σ vs cross-correlation length τ for various interface exponents $H_{1,2}$, $d=8$ nm, and correlation lengths $\xi_{1,2}=10$ nm.

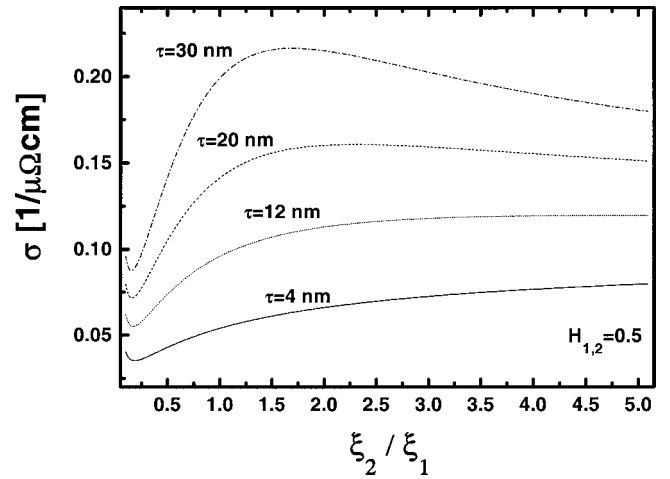


FIG. 3. Conductivity σ vs interface correlation length ratio ξ_2/ξ_1 with $\xi_1=10$ nm, $H_{1,2}=0.5$, $d=8$ nm, and various cross-correlation lengths τ .

fore the conductivity decreases with increasing correlation length $\xi_{1,2}$, while after some maximum point at $\xi_{1,2} \approx \lambda_F/4$ with further increment of the correlation length the conductivity increases since $\langle |h_{1,2}(q)|^2 \rangle \propto \xi_{1,2}^{-2H_{1,2}} (q\xi_{1,2} \gg 1)$. Such a minimum is more pronounced for one occupied miniband indicating that the interminiband transitions (for $N > 1$) will weaken such a scattering selectivity.

With increasing cross-correlation length τ a maximum of the conductivity develops for $\xi_2 > \xi_1$, as Fig. 3 shows, which becomes more pronounced for cross-correlation lengths τ significantly larger than the film/well thickness d . Such a maximum is also characterized by a steeper increment of the conductivity after passing its minimum for $\xi_2 > \lambda_F/4$. The conductivity increases in absolute magnitude with increasing cross-correlation length τ in agreement with Figs. 1 and 2. In addition, as a function of the roughness exponent H_2 , as Fig. 4 indicates, the conductivity increases with increasing H_2 (because scattering by roughness decreases) and increasing cross-correlation length τ . However, the degree of complexity is drastically reduced with respect to that shown in Fig. 3.

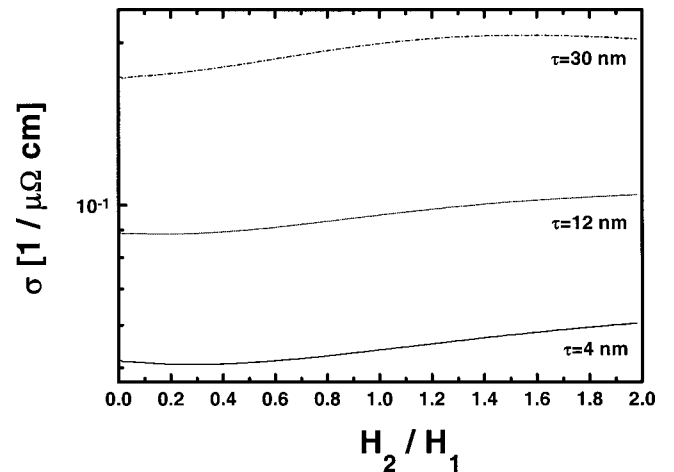


FIG. 4. Conductivity σ vs interface roughness exponent ratio H_2/H_1 with $H_1=0.5$, $\xi_{1,2}=10$ nm, $d=8$ nm, and various cross-correlation lengths τ .

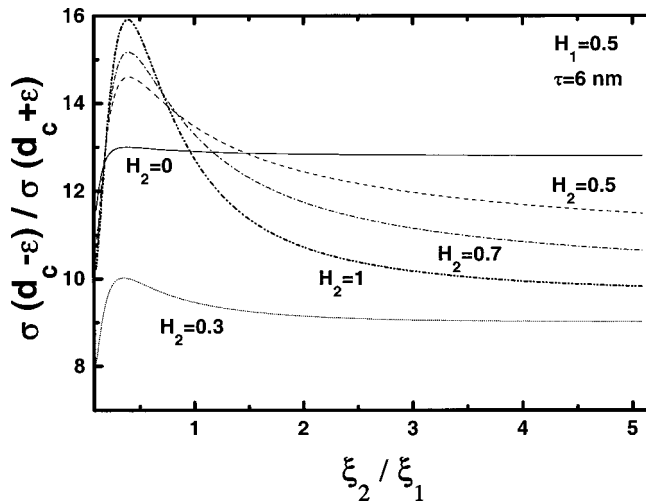


FIG. 5. Conductivity ratio vs interface correlation length ratio ξ_2/ξ_1 with $\xi_1 = 10$ nm, $d_c = 10$ nm, cross-correlation lengths $\tau = 6$ nm, and various interface roughness exponents $H_{1,2}$.

B. Conductivity ratio

In the following we shall concentrate on the conductivity ratio $\sigma(d_c - \epsilon)/\sigma(d_c + \epsilon)$, which is shown to depend sensitively on the form of the correlation function and as a result on the roughness exponents $H_{1,2}$.^{1–5} Note, however, that because $\langle |h_{1,2}(k)|^2 \rangle \sim \Delta_{1,2}^2$, the conductivity ratio $\sigma(d_c - \epsilon)/\sigma(d_c + \epsilon)$ is independent of the rms roughness amplitude as long as $\Delta_1 = \Delta_2$. Any complex dependence will arise predominantly from the interface roughness exponents $H_{1,2}$ and the in-plane roughness correlation lengths $\xi_{1,2}$. The numerical calculations were performed for $\epsilon = 0.1$ nm, and critical film/well thickness $d_c = 10$ nm (after which the Fermi level crosses the minimum of the second miniband).

In Fig. 5 we plot $\sigma(d_c - \epsilon)/\sigma(d_c + \epsilon)$ vs ξ_2/ξ_1 (with ξ_1 fixed) for various roughness exponents H_2 and $H_1 = 0.5$. For small correlation lengths $\xi_2 (\approx \lambda_F/4)$, the maximum of the conductivity ratio is very weak for small roughness exponents ($H_2 \approx 0$; close to logarithmic roughness) and becomes sharp for large roughness exponents $H_2 \approx 1$. For larger correlation lengths such that $\xi_2 > \xi_1$ ($\xi_1 > \lambda_F/4$), the conductivity ratio decreases with increasing roughness exponent H_2 as long as $H_2 > 0.5$. However, for small exponents $H_2 < 0.5$ the conductivity ratio increases with increasing roughness exponent H_2 . The latter indicates clearly the complex influence of the interface roughness exponents or alternatively of the form of the interface height–height correlation function.

In addition, in Fig. 6 we plot $\sigma(d_c - \epsilon)/\sigma(d_c + \epsilon)$ vs ξ_2/ξ_1 (with ξ_1 fixed) for various cross-correlation lengths τ and roughness exponents $H_{1,2} = 0.5$. The conductivity ratio exhibits a maximum at small correlation lengths ξ_2 ($\approx \lambda_F/4$) where the conductivity is minimum and further decreases with increasing ξ_2 . Nonetheless, such a maximum becomes strongly pronounced as long as the cross-correlation length τ becomes significantly larger than the film/well thickness d_c .

We should emphasize that the model for the conductivity includes the following simplifications: (i) The confining potential is infinite on both sides of the structure; (ii) the model

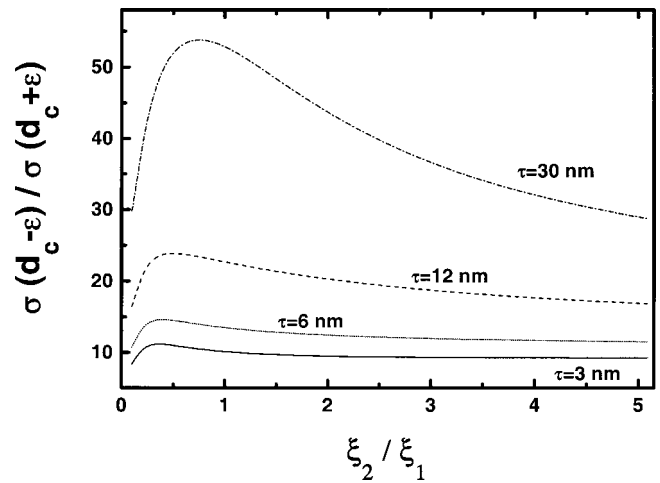


FIG. 6. Conductivity ratio vs interface correlation length ratio ξ_2/ξ_1 with $\xi_1 = 10$ nm, $H_{1,2} = 0.5$, $d_c = 10$ nm, and various cross-correlation lengths τ .

does not take into account electron scattering on impurities and/or other structural defects distributed inside the film. In a general case the situation is more complex, and these factors should also be considered. Furthermore, in some cases the boundary conditions on both sides of the film are significantly different and this asymmetry should also be taken into account. The influence of the confining potential on the electrical conductivity of single semiconducting films was already studied by Gottinger *et al.*,¹⁸ who showed that the weaker confining potential, the smaller surface contribution to the resistivity.

Finally, we should point out that the presence of cross correlations by means of Eq. (6) leads to increment of the conductivity. In general, the sign of the cross-correlation effect depends on certain model assumptions. This is because the cross correlation is an average of the product of inhomogeneities from opposite walls without having a predefined sign. The latter depends on the definition of the inhomogeneity distribution on both walls. For example, if someone follows the boundary wall definitions from Ref. 13 namely $z = \pm d/2 \mp h_{1,2}(\mathbf{r})$, then in Eq. (6) the cross-correlation term will have the opposite sign and thus will diminish the conductivity (see also Appendix).

VI. CONCLUSIONS

In this article we investigated surface/interface scattering effects on electrical transport properties of semiconducting thin films/quantum wells bounded by double random rough boundaries. The roughness was assigned to be of a random self-affine-type with an analytical roughness spectrum. Cross-correlation effects among the interfaces are taken into account during the conductivity calculations and are shown to strongly affect the electrical conductivity. Nonetheless, the exact effect depends on the particular values of the interface roughness exponents and correlation lengths. In addition, the conductivity ratio $\sigma(d_c - \epsilon)/\sigma(d_c + \epsilon)$, which depends sensitively on the form of the correlation function, is also strongly influenced by the presence of cross correlations.

ACKNOWLEDGMENTS

The authors would like to acknowledge support from The Netherlands Institute for Metals Research (NIMR) and useful discussions with Professor J. Barnas.

APPENDIX

The Hamiltonian that describes the system following the formalism of Fishman and Calecki¹ has the form

$$H = \frac{p_{xy}^2}{2m} + \frac{p_z^2}{2m} + V_1 \theta(-z - d/2 + h_1(\mathbf{r})) + V_2 \theta(z - [d/2 + h_2(\mathbf{r})]) \quad (\text{A1})$$

with $\theta(z)$ the step function, m the effective charge mass, $V_{1,2}$ the potential step height outside the well for $z > d/2$ and $z < -d/2$, P_{xy} the charge momentum in the $x-y$ plane where the motion is free, and P_z the charge momentum along the z direction where the motion is quantized. Expansion of the step functions in Eq. (A1) yields

$$\theta(-z - [d/2 + h_1(\mathbf{r})]) \approx \theta(-z - d/2) + h_1(\mathbf{r}) \delta(z + d/2), \quad (\text{A2})$$

$$\theta(z - [d/2 + h_2(\mathbf{r})]) \approx \theta(z - d/2) - h_2(\mathbf{r}) \delta(z - d/2), \quad (\text{A3})$$

which upon substitution in Eq. (A1) we obtain

$$H = H_o + V_1 h_1(\mathbf{r}) \delta(z + d/2) - V_2 h_2(\mathbf{r}) \delta(z - d/2), \quad (\text{A5})$$

$$H_o = \frac{p_{xy}^2}{2m} + \frac{p_z^2}{2m} + V_1 \theta(-z - d/2) + V_2 \theta(z - d/2), \quad (\text{A6})$$

with H_o the Hamiltonian for flat interfaces. The different signs in the second and third terms in Eq. (A5) is the origin of the $(-)$ sign in Eq. (6) for the cross-correlation term. This is clearly shown in the following calculation of the conductivity. Following Ref. 1, we have

$$\sigma = \frac{Sm^2 e^2}{\pi^2 \hbar^6 d} \sum_{n=1}^N \sum_{m=1}^N (E_F - E_n)(E_F - E_m) [C^{-1}(E_F)]_{nm} \quad (\text{A7})$$

$$[C(E_F)]_{nm} = \frac{2\pi}{\hbar} \sum_k \sum_{k'} \left[\delta_{nm} \sum_{\nu=1}^N |\langle nk|U|\nu k'\rangle|^2 k^2 \times \delta(E_F - E_{nk}) \delta(E_F - E_{\nu k}) - |\langle nk|U|mk'\rangle|^2 \times \mathbf{k} \cdot \mathbf{k}' \delta(E_F - E_{nk}) \delta(E_F - E_{mk}) \right], \quad (\text{A8})$$

where $U = V_1 h_1(\mathbf{r}) \delta(z + d/2) - V_2 h_2(\mathbf{r}) \delta(z - d/2)$. Calculation of the matrix elements $|\langle nk|U|mk'\rangle|^2$ yields¹

$$S|\langle nk|U|mk'\rangle|^2 = \sum_{b=1}^2 \tilde{A}_{nm}^b \int d^2 \mathbf{r} e^{-i(k' - k) \cdot \mathbf{r}} C_b(\mathbf{r}) - 2\tilde{B}_{nm} \int d^2 \mathbf{r} e^{-i(k' - k) \cdot \mathbf{r}} C_{12}(\mathbf{r}), \quad (\text{A9})$$

where $C_b(r) = \langle h_b(\mathbf{r}) h_b(\mathbf{0}) \rangle$ ($b = 1, 2$) is the height-height correlation function for each interface, and $C_{12}(r) = \langle h_1(\mathbf{r}) h_2(\mathbf{0}) \rangle$ the cross-correlation function. S is the average flat macroscopic interface area. From Eq. (A9) and Eqs. (A7) and (A8) follow the conductivity expressions.

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